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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

During the period covered by this report, the investigator continued his research on the development and application of numerical methods for singularly perturbed (or stiff) boundary value problems for ordinary differential equations. Results were obtained for collocation and finite difference methods for scalar and vector systems of two-point boundary value problems and for adaptive grid finite element methods for partial differential equations. His exponentially weighted finite element and spline in tension methods are being applied to partial differential equations as well as to ordinary differential equations

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INTERIM SCIENTIFIC REPORT

Air Force Office of Scientific Research Grant AFOSR-80-0192

Period: 1 June 1980 through 31 May 1981

Title of Research: Numerical Methods for Singularly Perturbed Differential Equations with Applications

Principal Investigator: Joseph E. Flaherty

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ABSTRACT

During the period covered by this report we continued our research on the development and application of numerical methods for singularly-perturbed (or stiff) boundary value problems for ordinary differential equations and initial-boundary value problems for partial differential equations. Results were obtained for collocation and finite difference methods for scalar and vector systems of two-point boundary value problems and for adaptive grid finite element methods for partial differential equations. Our exponentially weighted finite element and spline in tension methods are now being applied to partial differential equations as well as to ordinary differential equations.

1. Progress and Status of the Research on Numerical Methods for Singularly Perturbed Differential Equations

During the period covered by this report we continued our research on the development and application of numerical methods for singularly-perturbed ordinary and partial differential equations.

1.1 Boundary Value Problems for Ordinary Differential Equations

Our work on collocation with polynomial and tension splines for second order two-point boundary value problems has appeared in a sequence of two papers [1,3]*. This work has been extended to vector systems of boundary value problems and a paper describing the theoretical aspects of our work as well as some preliminary computational results has appeared in [2]. Additional computations have been performed and they indicate that our method offers significant advantages over existing techniques for two-point boundary value problems. Our findings are being incorporated into a report [6] which will be submitted for publication shortly.

The work on vector systems of ordinary differential equations [2,6] is joint research between Professors J. E. Flaherty and R. E. O'Malley, Jr. This grant supported this collaboration and Professor O'Malley visited Professor Flaherty at R.P.I. for about one month this year. In addition, Professor Flaherty visited Professor O'Malley at the University of Arizona for two weeks during the period of this report. Professor O'Malley joined R.P.I. in June, 1981 as Chairman of the Department of Mathematical Sciences, so travel funds will no

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*See the list of Publications and Abstracts at the end of this report.

longer be needed. The collaboration between Flaherty and O'Malley will, of course, continue.

In [5] Flaherty showed how our spline in tension methods [1,3] as well as certain exponentially weighted finite element methods could be made more efficient by using rational functions to approximate the required exponential functions. This paper also indicates how to extend these methods to partial differential equations.

1.2. Initial-Boundary Value Problems for Partial Differential Equations

A paper [4] describing our adaptive grid finite element procedure for initial-boundary value problems for vector systems of partial differential equations was published as an Institute for Computer Applications in Science and Engineering (ICASE) report and will subsequently appear in the SIAM Journal on Scientific and Statistical Computing. This work was based on the Ph.D Dissertation of S. F. Davis who was a graduate scholar under the direction of Professor Flaherty and who was supported by this grant. A second paper [8] based on Davis' thesis which describes some of the linear algebra algorithms is being prepared for publication.

Flaherty and a graduate student, J. M. Coyle, are working on several additions and improvements to our adaptive finite element code. These include local time step refinement routines and extensions to higher dimensions.

We are also extending our spline in tension methods to partial differential equations. We have begun by considering explicit finite difference and finite element methods for vector systems of hyperbolic and parabolic equations. These methods give sharp shocks, with no spurious diffusion or oscillations, without the need of a fine discretization. We presented some of our results at the Twenty-seventh Conference of Army Mathematicians, which was held at West Point, and our findings will appear in the proceedings of this meeting [7]. We will also submit them for publication in the open literature.

2. Interactions

Professor Flaherty was invited to lecture on material pertaining to this grant at the following conferences or organizations:

Conference on Boundary and Interior Layers (BAIL I), Trinity College, Dublin, Ireland, 3-6 June, 1980.

Workshop on Numerical Methods for Boundary Value Problems, University of British Columbia, Vancouver, British Columbia, 4-15 August, 1980.

American Mathematical Society, 780th Meeting, Special Session on Scientific Computing and Numerical Analysis, Brown University, Providence, Rhode Island, 18-19 October, 1980.

Department of Computer Science, Yale University, New Haven, Connecticut, 20 October, 1980.

Department of Computer Science, University of Waterloo, Waterloo, Ontario, 29 October, 1980.

Department of Computer Science, University of Toronto, Toronto, Ontario, 30 October, 1980.

Department of Mathematics, Old Dominion University, Norfolk, Virginia, 14 November, 1980.

Professor Flaherty was on sabbatical leave from R.P.I. during most of the period covered by this report and he visited the following laboratories and organizations and conducted research on the topics noted:

ICASE, NASA Langley Research Center, Hampton, Virginia, 30 September-10 October and 3-21 November, 1981. Performed research on adaptive grid finite element methods and lectured on the same as well as numerical methods for singularly-perturbed boundary value problems.

Program in Applied Mathematics, University of Arizona, 8-19 December, 1980. Conducted research with R. E. O'Malley, Jr. on numerical methods for singularly-perturbed systems of ordinary differential equations.

Benét Weapons Laboratory, Watervliet Arsenal, Watervliet, New York, 1 January, 1981-31 May, 1981. Conducted research on adaptive grid and exponentially weighted finite element methods. Applied these methods to wave propagation, impact, and penetration problems.

Terminal Ballistics Division, Ballistic Research Laboratory, Aberdeen Proving Ground, Maryland, 11-12 February, 1981. Discussed numerical techniques for impact and penetration problems with J. Zukas, Chief, Terminal Ballistics Division.

3. List of Publications and Manuscripts in Preparation

Publications

1. J. E. Flaherty and W. Mathon, "Collocation Methods for Singularly Perturbed Boundary Value Problems", in J. J. H. Miller, Ed., Boundary and Interior Layers - Computational and Asymptotic Methods, Boole Press, Dublin, 1980, pp. 77-92.

2. J. E. Flaherty and R. E. O'Malley, Jr., "On the Numerical Integration of Two-Point Boundary Value Problems for Stiff Systems of Ordinary Differential Equations," in J. J. H. Miller, Ed., Boundary and Interior Layers - Computational and Asymptotic Methods, Boole Press, Dublin, 1980, pp. 93-102.

3. J. E. Flaherty and W. Mathon, "Collocation with Polynomial and Tension Splines for Singularly Perturbed Boundary Value Problems", SIAM J. Sci. and Stat. Comp., Vol. 1 (1980), pp. 260-289.

In Press

4. S. F. Davis and J. E. Flaherty, "An Adaptive Finite Element Method for Initial-Boundary Value Problems", ICASE Report No. 81-13, ICASE, NASA Langley Research Center, Hampton, Virginia, March, 1981. Also, accepted for publication in SIAM J. Sci. and Stat. Comp., June, 1981.

5. J. E. Flaherty, "A Rational Function Approximation for the Integration Point in Exponentially Weighted Finite Element Methods", Tech. Rep. ARLCB-TR-81022, Benét Weapons Laboratory, Watervliet Arsenal, Watervliet, New York, June, 1981. Also, accepted for publication in Int. J. Num. Meth. Engng., June, 1981.

In Preparation

6. J. E. Flaherty and R. E. O'Malley, Jr., "Numerical Methods for Stiff Systems of Two-Point Boundary Value Problems", to appear as an ICASE Report, NASA Langley Research Center, Hampton, Virginia. Also to be submitted to SIAM J. Sci. and Stat. Comp.

7. J. E. Flaherty, "Explicit Difference Schemes for Wave Propagation and Impact Problems", to appear in Proc. Twenty-seventh Conf. of Army Mathematicians, USMA, West Point, New York, June, 1981. Also to be submitted to SIAM J. Sci. and Stat. Comp.

8. S. F. Davis and J. E. Flaherty, "A Stable Factorization of Block-Tridiagonal Matrices", to be submitted to <u>ACM Trans. Math. Software</u>.

COLLOCATION METHODS FOR SINGULARLY PERTURBED BOUNDARY VALUE PROBLEMS

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ABSTRACT

Collocation methods using both cubic polynomial and exponential splines are presented for second order singularly-perturbed two-point boundary value problems. Rules are presented for selecting tension parameters and collocation points. The methods converge outside of boundary layer regions without the necessity of using a fine discretization. Several numerical examples comparing the methods are presented

J. J. H. Miller, Ed., Boundary and Interior Layers - Computational and Asymptotic Methods, Boole Press, Dublin, 1980, pp.77-92.

ON THE NUMERICAL INTEGRATION OF TWO-POINT BOUNDARY VALUE PROBLEMS FOR STIFF SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

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and

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ABSTRACT

We consider a class of two-point boundary value problems for systems of the form $\dot{x} = f(x,y,t,\varepsilon)$, $\varepsilon\dot{y} = g_1(x,t,\varepsilon) + g_2(x,t,\varepsilon)y$ where the matrix $g_2(x,t,0)$ has a hyperbolic splitting with a fixed number of stable and unstable eigenvalues. Solutions to such boundary value problems can then be expected to have boundary layer behavior near both endpoints in the limit $\varepsilon \to 0^+$. We obtain uniform asymptotic representations of solutions. Our analysis shows, in particular, how to determine the reduced order boundary value problem satisfied by the limiting interior solution. Orthogonal matrix methods are used to determine this reduced problem and appropriate boundary layer corrections in a computationally effective manner. Numerical experiments with model problems illustrate the possibility of multiple solutions and show how our asymptotic results can be used in combination with the COLSYS code for solving two-point problems via collocation.

J. J. H. Miller, Ed., Boundary and Interior Layers - Computational and Asymptotic Methods, Boole Press, Dublin, 1980, pp. 93-102.

COLLOCATION WITH POLYNOMIAL AND TENSION SPLINES FOR SINGULARLY PERTURBED BOUNDARY VALUE PROBLEMS

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ABSTRACT

Collocation methods using both cubic polynomials and splines in tension are developed for second order linear singularly-perturbed two-point boundary value problems. Rules are developed for selecting tension parameters and collocation points. The methods converge outside of boundary layer regions without the necessity of using a fine discretization. Numerical examples comparing the methods are present.

SIAM J. Sci. & Stat. Comp., Vol. 1 (1980), pp. 260-289.

AN ADAPTIVE FINITE ELEMENT METHOD FOR INITIAL-BOUNDARY VALUE PROBLEMS FOR PARTIAL DIFFERENTIAL EQUATIONS

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and

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ABSTRACT

A finite element method is developed to solve initial-boundary value problems for vector systems of partial differential equations in one space dimension and time. The method automatically adapts the computational mesh as the solution progresses in time and is thus able to follow and resolve relatively sharp transitions such as mild boundary layers, shock layers, or wave fronts. This permits an accurate solution to be calculated with fewer mesh points than would be necessary with a uniform mesh.

The overall method contains two parts, a solution algorithm and a mesh selection algorithm. The solution algorithm is a finite element-Galerkin method on trapezoidal space-time elements, using either piecewise linear or cubic polynomial approximations and the mesh selection algorithm builds upon similar work for variable knot spline interpolation.

A computer code implementing these algorithms has been written and applied to a number of problems. These computations confirm that the theoretical error estimates are attained and demonstrate the utility of variable mesh methods for partial differential equations.

ICASE Report No. 81-13, ICASE, NASA Langley Research Center, Hampton, Virginia, March, 1981. Also, accepted for publication in SIAM J. Sci. and Stat. Comp., June, 1981.

A RATIONAL FUNCTION APPROXIMATION FOR THE INTEGRATION POINT IN EXPONENTIALLY WEIGHTED FINITE ELEMENT METHODS

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ABSTRACT

A rational function is presented for approximating the function $f(z) = \coth z - 1/z$ that appears in several exponentially fitted or weighted finite difference and finite element methods for convection-diffusion problems. The approximation is less expensive to evaluate than $f(z)$ and provides greater accuracy than the doubly asymptotic approximation when $z = O(1)$.

Tech. Rep. ARLCB-TR-81022, Benét Weapons Laboratory, Watervliet Arsenal, Watervliet, N.Y., June, 1981. Also, accepted for publication in INT. J. Num. Meth. Engng., June, 1981.

NUMERICAL METHODS FOR STIFF SYSTEMS OF TWO-POINT BOUNDARY VALUE PROBLEMS

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and

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ABSTRACT

We develop collocation methods for a class of singularly-perturbed two-point boundary value problems where the critical Jacobian has a hyperbolic splitting with a fixed number of stable and unstable eigenvalues. We use the asymptotic representation of the solution and a collocation method to construct an approximate solution. This solution can either be accepted or supplied as an initial guess to a two-point boundary value code, such as COLSYS, for further refinement.

To appear as an ICASE Report, NASA Langley Research Center, Hampton, VA and to be submitted to SIAM J. Sci. and Stat. Comp.

EXPLICIT DIFFERENCE SCHEMES FOR WAVE PROPAGATION AND IMPACT PROBLEMS

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ABSTRACT

Explicit finite difference and finite element schemes are constructed to solve propagation, shock, and impact problems. The schemes are of upwind difference type, but suffer less from the effects of numerical dispersion and diffusion than classical upwind schemes. The relationship of the new schemes to existing explicit schemes is analyzed and numerical results and comparisons are presented for several examples.

To appear in Proc. Twenty-seventh Conf. of Army Mathematicians, USMA, West Point, N.Y., June, 1981 and to be submitted to SIAM J. Sci. and Stat. Comp.

A STABLE FACTORIZATION OF BLOCK-TRIDIAGONAL MATRICES

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ABSTRACT

A stable Gaussian elimination algorithm is developed for block tridiagonal systems. The algorithm pivots both within and outside of blocks and reorders equations so as to minimize fill in.

To be submitted to ACM Trans. Matl. Software.

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